MODELING UNCERTAINTIES AND NEAR-ROAD $PM_{2.5}$: A COMPARISON OF CALINE4, CAL3QHC AND AERMOD

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Abstract

Background: Scientific evidence has shown an association between particulate matter exposure and adverse human health impacts. Accurately predicting near-road $PM_{2.5}$ concentrations is therefore important for project-level transportation conformity and health risk analyses.

Methods: This study assessed the capability and performance of three dispersion models, CALINE4, CAL3QHC, and AERMOD, in predicting near-road $PM_{2.5}$ concentrations. The comparative assessment included identifying differences among the three models in terms of methodology and data requirements. An intersection in Sacramento, California and a busy road in London, United Kingdom were used as sampling sites to evaluate how model predictions differed from observed PM2.5 concentrations.

Results: Screen plots and statistical tests indicated that, at the Sacramento site, CALINE4 and CAL3QHC performed moderately well, while AERMOD under-predicted $PM_{2.5}$ concentrations. For the London site, both CALINE4 and CAL3QHC resulted in over-predictions when incremental concentrations due to on-road emission sources were low, while under-predictions occurred when incremental concentrations were high. The street canyon effect and receptor location likely contributed to the relatively poor performance of the models at the London site.

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About The U.C. Davis-Caltrans Air Quality Project

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Mission: The Air Quality Project (AQP) seeks to advance understanding of transportation related air quality problems, develop advanced modeling and analysis capability within the transportation and air quality planning community, and foster collaboration among agencies to improve mobility and achieve air quality goals.

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1 Introduction

1.1 Problem Statement

Particulate matter (PM), also called particulates or fine particles, is a mixture of tiny solid and/or liquid particles. PM, especially those with a diameter less than or equal to 2.5 µm ($PM_{2.5}$), can be inhaled through the respiratory tract and cause adverse health impacts. Scientific evidence has shown a clear association between $PM_{2.5}$ and several human health problems. For example, Englert (Englert, 2004) and Kappos et al. (2004) reviewed the epidemiological studies for PM and concluded that long-term exposure to a high concentration of $PM_{2.5}$ increases the risk of acute and chronic respiratory infection, lung cancer, arteriosclerosis and other cardiovascular diseases, while short-term $PM_{2.5}$ exposure exacerbates existing pulmonary and cardiovascular diseases. To better protect public health, in 2006 the US Environmental Protection Agency (EPA) revised the 24-hour $PM_{2.5}$ standard from 65 µg/m^3 to 35 µg/m^3 (USEPA, 2006).

The composition of $PM_{2.5}$ may change temporally and spatially; therefore, its toxicity varies. $PM_{2.5}$ from vehicle emissions is associated with adverse health problems (Adar et al., 2007; Kim et al., 2004; Kok et al., 2006; Ryan et al., 2007; Tonne et al., 2007; Vliet et al., 1997). Brugge (2007) estimated that, "approximately 11% of US households are located within 100 meters of 4-lane highways", where vehicle emissions are the major source of $PM_{2.5}$. Because monitoring $PM_{2.5}$ concentrations cannot be done for all near-road regions, using appropriate models with vehicle and meteorological information to estimate near-road $PM_{2.5}$ concentrations is essential.

1.2 Study Objectives

Air dispersion models used to estimate gas concentrations are used for predicting near-road particle concentrations. In this study, the capabilities and features of three dispersion models, CALINE4, CAL3QHC and AERMOD, are evaluated. Specifically, the research objectives are to examine the performance of the three models individually based on their predictions of $PM_{2.5}$ concentrations at two sites, an intersection of Florin Road and Stockton Boulevard in Sacramento, California and a busy road in London, United Kingdom. Hypotheses, such as whether the model over or under-predicts the concentrations, whether the model under-prediction increases with observed concentration, and whether the three models are significantly different, are tested. The research aims to identify the models that are appropriate for predicting near-road $PM_{2.5}$ concentrations.

1.3 Organization of the Report

This report consists of six chapters and one appendix. Chapters 1 and 2 introduce the research background, clarify the study objectives and review previous related studies. Chapter 3 introduces and compares the three models from the theoretical perspective. Chapters 4 and 5 evaluate the three models through their performances at two sites. Chapter 6 summarizes the major results of this study and discusses future research. The appendix provides step-by-step instructions to run the three models.

2 Literature Review

2.1 Negative Impact of $PM_{2.5}$ and the Role of Vehicle $PM_{2.5}$ Emissions

Studies show a relationship between PM exposure and adverse human health impacts, regarding fine particles ($PM_{2.5}$), as well as coarse particles ($PM_{2.5-10}$). The US EPA, in the report "Particulate Matter Research Program: Five Years of Progress" (2004b), reviewed critical studies of PM and found that ambient $PM_{2.5}$ exposure is associated with morbidity and mortality caused by respiratory and cardiovascular diseases.

Because $PM_{2.5}$ is a complex mixture of organic and inorganic components, its composition varies temporally and spatially. Jerrett and Finkelstein (2005) showed that the toxicity of $PM_{2.5}$ varies for different States throughout the United States. Davidson et al. (2005) showed that health problems are associated with particle size and composition. Schlesinger (2007) examined the toxicity of common inorganic components of $PM_{2.5}$ and found clear adverse biological effects from some secondary acidic sulfates. He also indicated that different components were responsible for different adverse health outcomes.

Research has also shown that $PM_{2.5}$ that originated from vehicle emissions falls in the toxic category (Kok et al., 2006). Adar et al. (2007) conducted a study in suburban St. Louis, Missouri for elders and found a negative association between $PM_{2.5}$ and heart rate variability; the short-term association was mainly limited to traffic-related $PM_{2.5}$ rather than $PM_{2.5}$ from other sources. Other studies showed a relationship between near-highway $PM_{2.5}$ and childhood asthma, lung cancer, myocardial infarction and other health problems (Kim et al., 2004; Ryan et al., 2007; Tonne et al., 2007; Vineis, 2006). Therefore, knowing the $PM_{2.5}$ concentrations in regions near motorways is essential.

2.2 Dispersion Models – Brief Literature Review

There are various gas dispersion models. Holmes and Morawska (2006) reviewed previous studies which measured both gas and PM concentrations at the same time and concluded that gas and PM concentrations correlated quite well in an open environment.

The most widely used air dispersion models are the Gaussian models, which are based on two modified Gaussian distributions of the plume in the vertical and horizontal directions. Three Gaussian models, CALINE4, CAL3QHC and AERMOD, are used to predict near-road $PM_{2.5}$ concentrations in this study. CALINE4 has been widely used in California to evaluate transportation project-level air quality impacts; CAL3QHC is designed for carbon monoxide (CO) and PM concentrations and is one model suggested by EPA for dispersion modeling; AERMOD is an additional EPA-recommended model for dispersion modeling. All three models have been widely used to model gaseous pollutants. They have also been used to model PM concentrations in some limited applications.

2.2.1 CALINE4

The CALINE4 model is widely used to predict near-road vehicle emissions. This model has been tested and validated for predicting concentrations of several vehicle-emitted pollutants near-road under certain conditions, such as CO, oxides of nitrogen (NOx), and additional gases.

Loranger et al. (1995) showed that CALINE4 predicted near-road CO concentrations well, but under-predicted manganese (Mn) concentrations. Broderick et al. (2005) examined CALINE4's performance of modeling transportation-related CO for a free-flowing motorway and a periodically congested roundabout in Ireland and concluded that CALINE4 functioned well under stable atmospheric conditions but performed poorly under low wind conditions.

Marmur and Mamane (2003) showed that CALINE4, together with emission factors predicted by COPERT III, is suitable for near-road NOx concentration prediction in open urban and rural sites in Israel, though this conclusion may not be extended to dense urban center locations. Levitin et al. (2005) showed that CALINE4 performed well for near-road NOx and nitrogen dioxide (NO_2) concentrations prediction. Kenty et al. (2007) showed CALINE4 predicts NOx concentration well, but under-predicts NO_2 concentrations probably due to assumptions imbedded in the model.

Jones et al. (1998) showed that CALINE4 predicts well for daytime 12-hour average concentrations of transportation related benzene, toluene, ethylbenzene and xylene in urban areas. Broderick and O'Donoghue (2007) examined CALINE4's capability in predicting transportation related emissions of seven inert gases – *n*-Pentane, *Iso*-pentane, Ethene, Propene, 1,3-Butadiene, Acetylene and Benzene under low wind speeds and showed that CALINE4, together with emission factors predicted by COPERT III, gives good long-term estimations but underestimates higher percentile concentrations when evaluating short-term conditions.

CALINE4 has also been tested in predicting particle concentrations in two studies. Gramotnev et al. (2003) used a modified version of CALINE4 to estimate motor vehicle emission factors of fine and ultrafine particles near a busy road in the Brisbane area in Australia. Employing the resulting emission factors, they found that the CALINE4 model results matched the observed rate of dispersion with distance from the road well. Findings in the second study were mixed: CALINE4 performed well for an intersection in Sacramento site but not for urban road in London site (Yura et al., 2007) [note that this study reevaluates the same sites examined by Yura et al.].

2.2.2 CAL3QHC

CAL3QHC is designed for CO and PM concentration prediction. Studies to date on model performance have been mixed. Moseholm et al. (1996) showed that CAL3QHC yielded unsatisfying results under conditions involving low wind speeds and nearby tall buildings. Not unsurprisingly, Zhou and Sperling (2001) note that mixed traffic (bicycles and vehicles) and near-road high-rise buildings will cause CAL3QHC to poorly predict CO concentrations. An extensive evaluation of the CAL3QHC model was provided in a National Cooperative Highway

Research Program study (Carr et al., 2002) as part of the development of the Hybrid Roadway Intersection model (HYROAD). This report documents poor model performance at ten sites across the country, 3 where intensive CO monitoring was conducted plus an additional 7 with less intensive monitoring. However, CAL3QHC was shown to perform well generally in open areas with moderate traffic volumes (Abdul-Wahab, 2004) and along moderately trafficked suburban roads (Kho et al., 2007). CAL3QHC has also been used with somewhat less success to estimate both transportation-related $PM_{2.5}$ and PM_{10} (Gokhale and Raokhade, 2008) – in which the predicted concentrations did not match the measured concentrations well. PM dispersion from non-traffic sources may have been a main contributor to this mismatch.

2.2.3 AERMOD

AERMOD can be used for predicting the concentrations of various pollutants emitted by point, line and area sources. This model is typically used for large areas (Faulkner et al., 2007; Hanna et al., 2006; Jampana et al., 2004; Kumar et al., 2006; Stein et al., 2007; Touma et al., 2007) or stationary sources (Orloff et al., 2006; Seigneur et al., 2006). Kesarkar et al. (2007) used AERMOD to estimate PM_{10} concentrations over the city Puna in India and found that the model generally underestimated PM_{10} concentrations except for residential areas. Zhang et al. (2008) used AERMOD to estimate PM_{10} concentrations in the urban area of Hangzhou, China and found that AERMOD underestimated concentrations; the authors noted that model performance may have been related to lack of consideration of construction and secondary particles. Although the model has not been widely used in predicting near-road pollutant concentrations, EPA recommends AERMOD to evaluate near-road concentrations (USEPA, Accessed July 10, 2008) and thus it is included in this study.

2.2.4 PM Prediction by Other Models

There are other models that have been used to predict $PM_{2.5}$ or PM_{10} concentrations. Gokhale and Raokhade (2008) used CALINE3 and the 'Modified General Finite Line Source Model' (M-GFLSM) to estimate transportation related $PM_{2.5}$ and PM_{10} concentrations and found that both of them performed worse than CAL3QHC generally. Vardoulakis et al. (2007) used three dispersion models, WinOSPM (a Windows-based version of OSPM), ADMS-Urban 2.0 and AEOLIUS Full, to estimate vehicle PM_{10} emissions from two streets in Birmingham and London for one year and the models gave good estimates for PM_{10}. The reason for the good match partly relies on the high percentage of background concentration, which comprises approximately 80% of the total PM_{10} concentration. Bowker et al. (2007) used the 'Quick Urban and Industrial Complex' (QUIC) model to estimate the concentration of ultra fine particles near I-440 in Raleigh, North Carolina, and found that the predicted concentrations have a similar pattern to the measured concentrations.

3 Model Description

CALINE4, CAL3QHC and AERMOD are all Gaussian models. They are based on two modified Gaussian distributions of the plume in the vertical and horizontal directions. In addition, all three models are steady-state models; that is, the models assume that the dispersion process takes no time to achieve the steady state. The material and equations presented in this chapter are based on available model documentation.

3.1 CALINE4

CALINE4 is the most recent version of the CALINE model series developed by the California Department of Transportation. It embeds the concept of mixing zone and uses modified Gaussian distributions (Benson, 1984). CALINE4 uses a series of equivalent finite line sources to represent the road segment, and models the whole region of finite line sources as a zone with uniform emissions and turbulence. The concentration at a point with coordinates (x, y, z) is calculated based on equation (3-1).

$$C(x,y,z) = \frac{q}{2\pi u \sigma_y \sigma_z}\left\{\exp\left[\frac{-(z-H)^2}{2{\sigma_z}^2}\right] + \exp\left[\frac{-(z+H)^2}{2{\sigma_z}^2}\right]\right\}\int_{-y_1}^{y_2} \exp\left(\frac{-y^2}{2{\sigma_y}^2}\right)\, dy \qquad (3\text{-}1)$$

where q is the linear source length, u is the wind speed, σ_y and σ_z are the horizontal and vertical Gaussian dispersion parameters, H is the source height, y_1 and y_2 are the y -coordinates of finite line source endpoints.

Among all the variables, σ_y is a function of the x -coordinate of the point where the concentration is calculated and horizontal wind angle standard deviation; σ_z is modified by incorporating the effects of vehicle-induced heat.

3.2 CAL3QHC

CAL3QHC is an enhanced version of CALINE3 with an additional algorithm that estimates the lengths of vehicular queues at signalized intersections (USEPA, 1995). Thus, CAL3QHC can incorporate the emissions from idling vehicles as well as free-flow traveling vehicles; although the idling portion of the model was not evaluated as part of this study (refer to section 4.3). The dispersion process formulated in CAL3QHC is the same as that in CALINE4 by applying equation **(3-1)**. However, CAL3QHC uses atmospheric stability to estimate the horizontal dispersion parameter (σ_y), and the vertical dispersion parameter (σ_z) is not modified by the vehicle-induced heat algorithm (Benson, 1992).

3.3 AERMOD

AERMOD incorporates the concept of planetary boundary layer (PBL) (USEPA, 2004a) – the lowest part of the atmosphere and its characteristics that are directly affected by the earth's surface. There are two types of PBL: Stable Boundary Layer (SBL) and Convective Boundary Layer (CBL). SBL occurs when the earth's surface is colder than the air above, usually during the night; and CBL otherwise. Whether the PBL is SBL or CBL, and the parameters of the boundary layers, are determined by AERMET, a meteorological preprocessor used with AERMOD.

In SBL, two independent horizontal and vertical Gaussian distributions are used for modeling pollutant dispersion, the same as is used in CALINE4 and CAL3QHC. In CBL, the horizontal distribution is still Gaussian; however, the vertical distribution is a bi-Gaussian distribution (Cimorelli et al., 2005) and the concentration is calculated as a weighted average of two Gaussian distributions; this is the main difference between AERMOD and CALINE4/CAL3QHC. The concentration at a point with coordinates (x, y, z) is calculated based on equation (3-2):

$$C_T(x, y, z) = f \cdot C_{c,s}(x, y, z) + (1 - f) \cdot C_{c,s}(x, y, z_p) \tag{3-2}$$

where $C_{c,s}(x, y, z)$ and $C_{c,s}(x, y, z_p)$, with the subscripts c and s refer to convective and stable conditions, respectively, and denote the pollutant from the horizontal plume state and the terrain-following state, respectively, where z is the height of the point above stack base and z_p is the height of the point above local ground, and f is the plume state weighting function, calculated based on equation (3-3):

$$f = 0.5\left(1 + \frac{\int_0^{H_c} C_s(x, y, z)dz}{\int_0^{\infty} C_s(x, y, z)dz}\right) \tag{3-3}$$

where H_c is the critical dividing streamline height.

$C_s(x, y, z_*)$ can be calculated based on equation (3-4), where z_* can be either z or z_p:

$$C_s(x, y, z_*) = \frac{Q}{2\pi\pi u\sigma_y\sigma_{zs}} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) \times \sum_{m=-\infty}^{\infty}\left\{\exp\left[\frac{-\left(z_* - h_{es} - 2mz_{ieff}\right)^2}{2\sigma_{zs}^2}\right] + \exp\left[\frac{-\left(z_* + h_{es} + 2mz_{ieff}\right)^2}{2\sigma_{zs}^2}\right]\right\} \tag{3-4}$$

where Q is the source emission rate, u is the effective wind speed, σ_y is the horizontal Gaussian dispersion parameter, which is a function of non-dimensional distance, σ_{zs} is the total vertical dispersion parameter, h_{es} is the plume height, and z_{ieff} is the effective mechanical mixing height.

$C_c(x,y,z_*)$ can be calculated as shown in equation (3-5), where z_* can be either z or z_p:

$$C_c(x,y,z_*) = C_d(x,y,z_*) + C_r(x,y,z_*) + C_c(x,y,z_*) \qquad (3\text{-}5)$$

where $C_d(x,y,z_*)$, $C_r(x,y,z_*)$, and $C_c(x,y,z_*)$ denote pollutants from direct, indirect and penetrated sources, respectively. They are calculated based on equations (3-6), (3-7) and (3-8), respectively:

$$C_d(x,y,z_*) = \frac{Qf_p}{2\pi\pi u\sigma_y}\exp\left(\frac{-y^2}{2\sigma_y^2}\right) \times \sum_{j=1}^{2}\sum_{m=0}^{\infty}\frac{\lambda_j}{\sigma_{zj}}\left\{\exp\left[\frac{-(z_* - \Psi_{dj} - 2mz_i)^2}{2\sigma_{zj}^2}\right] + \exp\left[\frac{-(z_* + \Psi_{dj} + 2mz_i)^2}{2\sigma_{zj}^2}\right]\right\} \qquad (3\text{-}6)$$

where f_p is the fraction of source material that remains trapped in the CBL, Ψ_{dj} and σ_{zj} are the effective source height of the direct source and vertical dispersion parameter, with j equals to 1 or 2 corresponding to each of the Gaussian distribution used in the bi-Gaussian distribution, λ_j is the weighting coefficient for each of the distribution, with λ_1 and λ_2 sum to 1, and z_i is the mixed layer height in the CBL;

$$C_r(x,y,z_*) = \frac{Qf_p}{2\pi\pi u\sigma_y}\exp\left(\frac{-y^2}{2\sigma_y^2}\right) \times \sum_{j=1}^{2}\sum_{m=0}^{\infty}\frac{\lambda_j}{\sigma_{zj}}\left\{\exp\left[\frac{-(z_* + \Psi_{rj} - 2mz_i)^2}{2\sigma_{zj}^2}\right] + \exp\left[\frac{-(z_* - \Psi_{rj} + 2mz_i)^2}{2\sigma_{zj}^2}\right]\right\} \qquad (3\text{-}7)$$

where Ψ_{rj} is the effective source height of the indirect source, and other parameters are the same as in equation (3-6);

$$C_p(x,y,z_*) = \frac{Q(1-f_p)}{2\pi\pi u\sigma_y\sigma_{zp}}\exp\left(\frac{-y^2}{2\sigma_y^2}\right) \times \sum_{m=-\infty}^{\infty}\left\{\exp\left[\frac{-(z_* - h_{ep} - 2mz_{ieff})^2}{2\sigma_{zp}^2}\right] + \exp\left[\frac{-(z_* + h_{ep} + 2mz_{ieff})^2}{2\sigma_{zp}^2}\right]\right\} \qquad (3\text{-}8)$$

where σ_{zp} is the vertical dispersion coefficient, h_{ep} is the source height of the penetrated source, and other parameters the same as in equations (3-4) and (3-6).

3.4 Data Requirements

To estimate near-road $PM_{2.5}$ concentrations, all three models need vehicle-related data, meteorological information and data such as link geometry and receptor locations (see Table 3-1). Vehicle-related data mainly include traffic volumes and vehicle emission factors. They are used as direct inputs in CALINE4 and CAL3QHC, and they are used to calculate source emission rates together with source type and geometry information in AERMOD. CAL3QHC has a queue algorithm as an optional function, which requires additional traffic data.

CALINE4 and CAL3QHC have almost the same requirements for meteorological data, while AERMOD requires much more detailed meteorological information. For example, AERMOD requires upper air sounding data including atmospheric pressure, dry bulb temperature, dew-point temperature, and wind direction and wind speed at several levels above sea level. Ideally, when ample meteorological data are available, AERMOD may replicate atmospheric conditions better than CALINE4 or CAL3QHC. However, AERMOD also increases the complexity of model runs and parameter specifications due to relatively intensive data needs.

Table 3-1 Data Requirements of CALINE4, CAL3QHC, and AERMOD

	CALINE4	CAL3QHC	AERMOD
Vehicle-Related Data			
Traffic Volume	√	√	√
Emission Factor	√	√	√
Average Total Signal Cycle Length		■	
Average Red Total Signal Cycle Length		■	
Clearance Lost Time		■	
Approach Volume on the Queue Link		■	
Idle Emission Factor		■	
Saturation Flow Rate		■	
Arrival Rate		■	
Meteorological Data			
Wind Speed	√	√	√
Wind Direction	√	√	√
Wind Direction Variation	√	Δ	
Dry Bulb Temperature	√	√	√
Wet Bulb Temperature			Δ
Dew-Point Temperature			Δ
Atmospheric Stability Class	√	√	
Surface Roughness	√	√	√
Midday Albedo			√
Daytime Bowen Ratio			√
Total/Opaque Sky Cover			√
Sky Cover at layer 1,2,3,4			Δ
Relative Humidity			Δ
Precipitation Amount			Δ
Precipitation Type			Δ
Horizontal Visibility			Δ
Cloud Type			Δ
Sea Level Pressure			Δ
Station Pressure			Δ
Upper Air Sounding			√
Other Data			
Source Height	√	√	√
Mixing Zone Width	√	√	√
Link Geometry	√	√	√
Receptor Coordinates	√	√	√
Settling Velocity	√	√	
Deposition Velocity	√	√	
Longitude and Latitude			√

Where: √ = required input; Δ = optional input; ■ = required for CAL3QHC's queue algorithm.

4 Case Study – Background and Model Setup

4.1 Study Area

Data from two sampling sites are used to evaluate the capabilities of the three models in this study. One is the intersection at Florin Road and Stockton Boulevard in Sacramento, California (see Figure 4-1); the other is on Marylebone Road, London (see Figure 4-2).

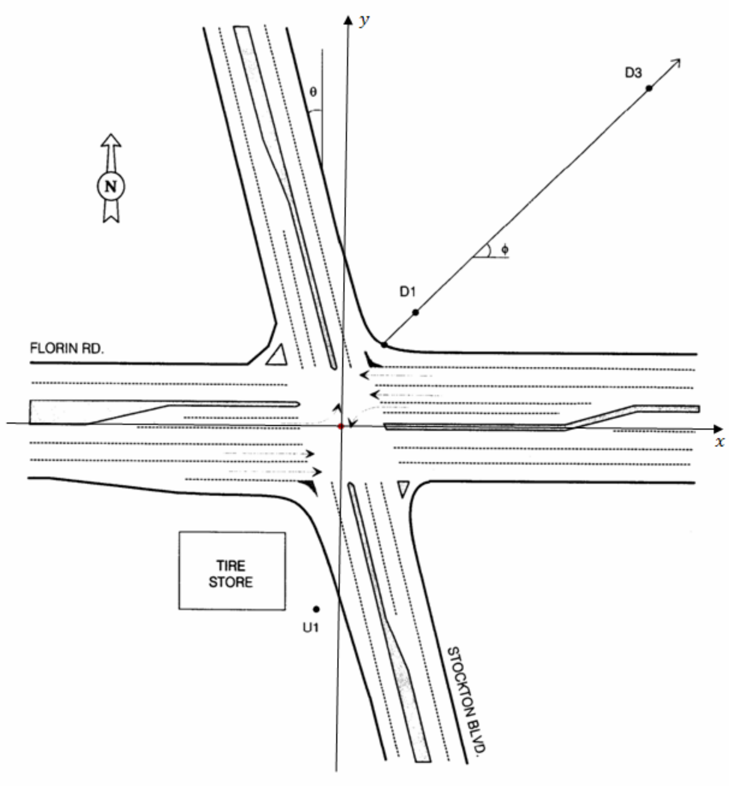


Figure 4-1 Sacramento Site Layout

Adapted from Vicente J. Garza (Ashbaugh et al., 1996).

There are three receptors, two at location D1 with the height of 3m and 9m, respectively, and one at D3 with the height of 3m. In the reference frame shown in the figure, the x,y – coordinates of D1 and D3 are (18.3m, 19.4m) and (74.5m, 75.6m), respectively. The two angles are 16° for θ and 45° for ϕ.

Florin Road has seven lanes and its width is 26m. Stockton Boulevard has six lanes and its width is 22m. Both links extended 150m (Ashbaugh et al., 1996) from the center of the intersection and are considered in the model analyses, i.e., two links of 300m. By convention, if there is no immediate barrier at sides of the road, the region within 3m at each side of the road is also considered as the emission source (Benson, 1984, pp.160). Therefore, two rectangles are considered as sources in this situation. The area of the Florin Road rectangle is 300m times 32m, with the coordinates of the four corners being (-150m, -16m), (-150m, 16m), (150m, 16m) and (150m, -16m). The area of the Stockton Boulevard rectangle is 300m times 28m, with the coordinates of the four corners (-27.9m, 148.0m), (-54.8m, 140.3m), (27.9m, -148.0m) and (55.8m, -140.3m) (see reference x-y axis frame shown in Figure 4-1).

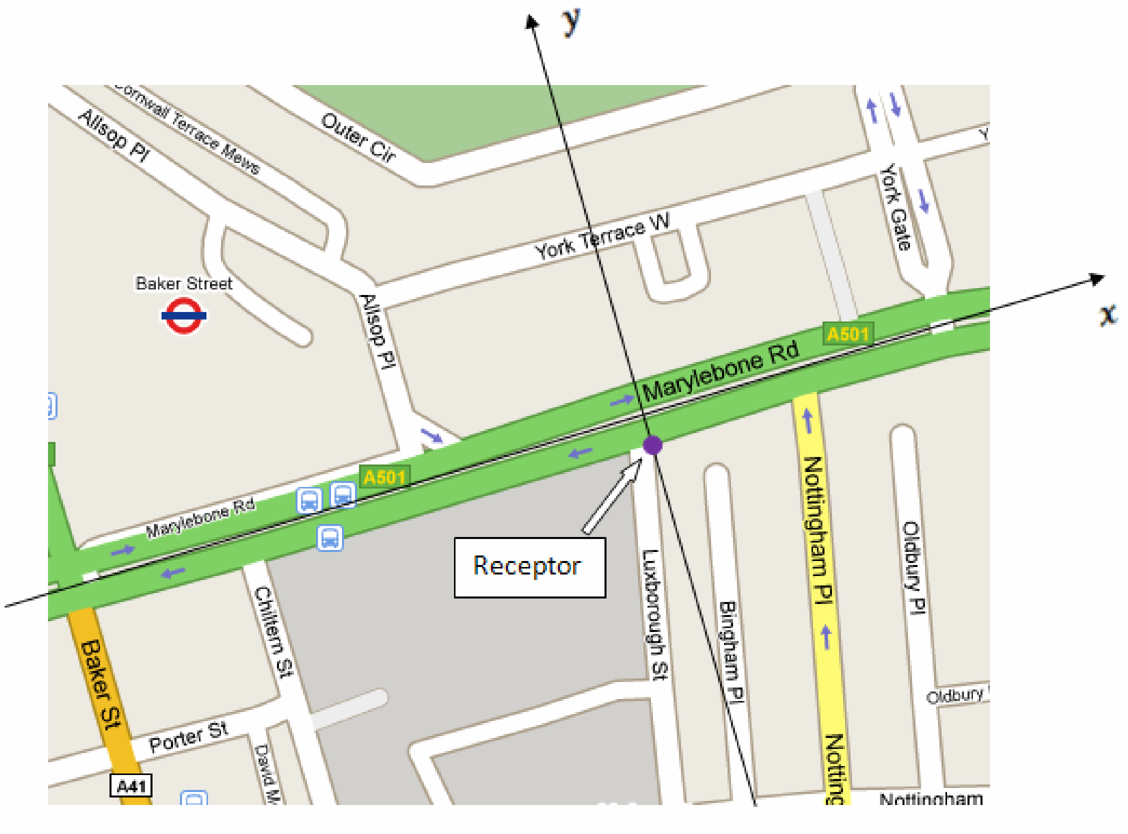


Figure 4-2 London Site Layout

From http://maps.google.com.

The reference frame is shown in the figure. The receptor's coordinates in the reference frame is (0, -13.5m), and the receptor's height is 3m.

Marylebone road has six lanes with a width of 22m. The link extending 200m (Yura et al., 2007) from the origin is considered in the models; that is, 400m in total. Similarly, as in the Sacramento site, 3m at each side of the road is also considered as part of the source. Therefore, the source rectangle considered in the model is of area 400m times 28m and with the coordinates of the four corners (-200m, -14m), (-200m, 14m), (200m, 14m) and (200m, -14m) in the reference frame shown in Figure 4-2.

4.2 Observed $PM_{2.5}$ Concentrations

For the Sacramento site, observed concentrations from ten time periods were compared with model predictions. Table 4-1 shows the background $PM_{2.5}$ concentration, as well as the increment, which is the concentration observed at the receptor minus the background concentration. The background concentrations vary by time period only; for a given time period, background is assumed to be the same at different locations. The increments reflect the effect of traffic-related $PM_{2.5}$ emissions on the receptors.

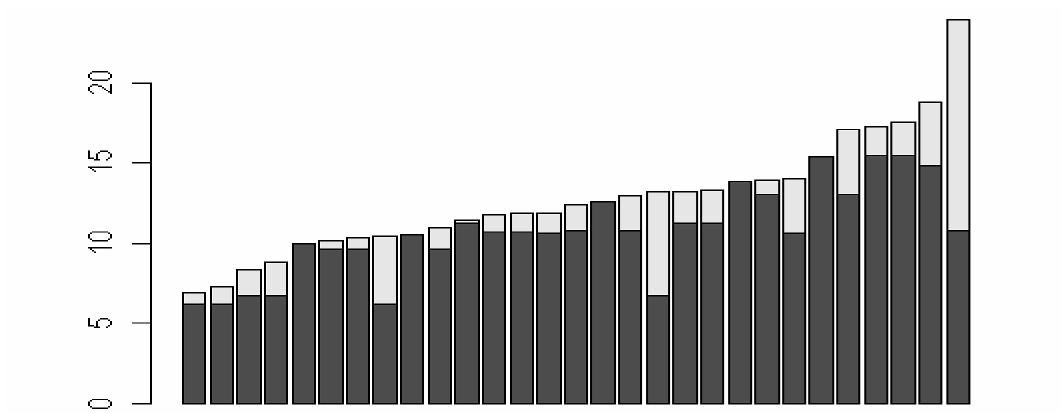
Table 4-1 $PM_{2.5}$ Concentrations ($\mu g/m^3$) at the Sacramento Site

ID	Time	Background concentration	Increment at D1 (3m)	Increment at D1 (9m)	Increment at D3 (3m)
1	8/23 12:00 – 16:00	6.245	4.225	0.685	1.065
2	8/23 16:00 – 19:00	6.765	6.435	1.575	2.085
3	8/24 6:00 – 10:01	13.07	4	0	0.84
4	8/24 11:43 – 16:00	10.8	13.1	1.59	2.17
5	8/24 16:00 – 20:55	10.635	3.355	1.265	0
6	8/24 20:55 – 8/25 5:55	15.43	2.11	0	1.8
7	8/25 5:55 – 10:01	14.8	4.02	0	8.03[i]
8	8/25 21:00 – 8/26 5:56	10.68	1.08	0	1.17
9	8/26 5:56 – 10:00	11.275	1.985	0.175	2.005
10	8/26 16:06 – 19:00	9.67	1.27	0.48	0.66

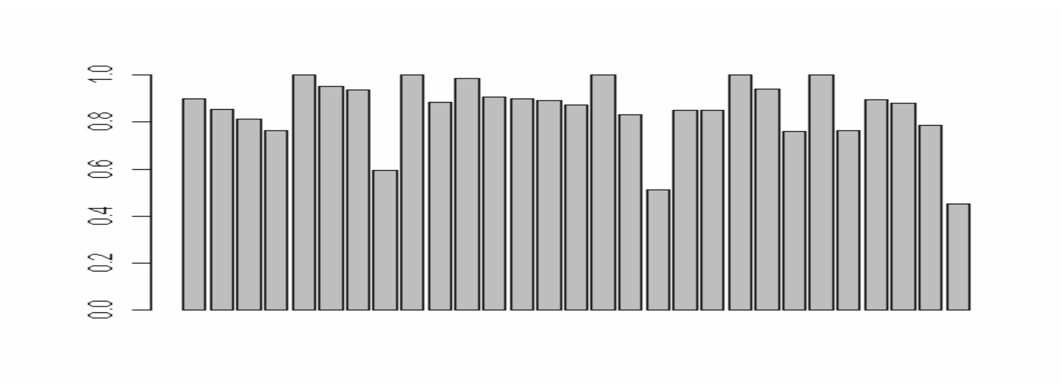
Source: the above table uses information available from Ashbaugh et al.'s paper (1996).

[i]: This data is considered to be a measurement error. The reason is that it is much larger than the increment concentration at D1(3m) at the same time period, and much larger than the increment concentrations at D3(3m) at other time periods. This data point is not used in the model evaluation.

Data in Table 4-1 suggest that the increments are relatively small compared with the background concentrations. The background proportion exceeds 70% for most samples, regardless of the value of the total concentration (see Figure 4-3). Since the models estimate the incremental concentration directly, the large background concentrations will tend to improve model performance when total concentrations are considered (background plus increment). Therefore, the comparison was conducted for both with-background and without-background scenarios.



(a)



(b)

Figure 4-3 Background Proportion Plots (Sacramento Case)
(a) The whole bar is the total PM2.5 concentration and the dark part is the background concentration. (b) The corresponding background proportion among the total concentration. For both plots, samples are in the order of increasing total concentration.

For the London site, observed concentrations from 253 hours during the time period from July 31, 1998 to July 17, 2000, are used. The data are selected based on associated meteorological information (Yura et al., 2007). Similarly as in the Sacramento case, the increments are also relatively small when compared with the background concentrations. Therefore, as with the Sacramento case study, concentrations with and without background are considered in the model comparisons.

4.3 Model Inputs

Because detailed intersection information (e.g., signal data, idling emissions, and traffic delays) is unavailable for both sites, the queuing algorithm embedded in the CAL3QHC model was not used. In addition, AERMOD was not used for the London site, because upper air sounding data and sky cover information were lacking for the monitoring events.

The surface roughness is set to be 100cm for both sites since they are in urban areas. The midday Albedo and daytime Bowen ratio required for AERMOD are set to be 0.16 and 2.0, respectively, according to AERMOD's User Guideline (USEPA, 2004c). Two important parameters are discussed below.

4.3.1 Emission Factor (EF)

Two methods were used for quantifying emission factors. In the Sacramento case, a steady-state box model was used. The model assumes a virtual box over the road segment and the pollutant concentration is uniform inside the box. The emission factor is calculated as shown in equation (4-1):

$$EF = \frac{3.6 \times u \times h \times C \times cos\theta}{N} \quad (4\text{-}1)$$

where u is the wind speed (m/s), h is the height of the mixing box (m), C is the measured pollutant concentration (μg/m^3), θ is the wind direction (degrees), N is the number of vehicles per hour, and the calculated emission factor is of the unit of gram per vehicle kilometer traveled (g/VKT) (Ashbaugh et al., 1996). The box model is used in the Sacramento case so that the calculated emission factors reflect both free-flow and idling vehicle emissions.

In the London site, the emission factor is calculated as a weighted average over different vehicle categories as shown in equation (4-2). The emission factors of light-duty vehicles and heavy-duty vehicles are shown in Table 4-2:

$$EF = \frac{EF_{LD} \times N_{LD} + EF_{HD} \times N_{HD}}{N_{LD} + N_{HD}} \quad (4\text{-}2)$$

where the subscripts LD and HD denote 'light-duty vehicle' and 'heavy-duty vehicle', respectively, and N is the vehicle number.

Table 4-2 Emission factors of PM2.5 (g/VKT)

Year	1998	1999	2000
Light-duty vehicle	0.0268	0.0260	0.0225
Heavy-duty vehicle	0.418	0.358	0.279

Source: (Yura et al., 2007).

4.3.2 Deposition and Settling Velocities

$PM_{2.5}$ can be removed from the atmosphere by dry deposition, precipitation scavenging, and/or chemical reactions. In both case studies, models are used on days without precipitation and we also do not consider the chemical reactions of $PM_{2.5}$; only dry deposition is considered.

Dry deposition is mainly due to gravitation, turbulent diffusion and Brownian motion (Hanna et al., 1982, pp 67-71). By Stokes' law, the terminal settling speed (v_t), which is due to gravitation, can be calculated based on equation (4-3):

$$v_t = \frac{2r^2 g\rho}{9\mu} \tag{4-3}$$

where r is the particle radii, ρ is particle density, and μ is dynamic viscosity of air ($1.8 \times 10^{-4} g/(s \cdot cm)$). In the two case studies, the concentration of $PM_{2.5}$ is estimated, so the particle radii is no more than 1.25 µm, also the particle densities are no more than 60 µg/m^3 in both case studies, so the calculated terminal settling speed is no more than $1.13 \times 10^{-12} cm/s$, which is very small and is negligible. The dry deposition by turbulent diffusion and Brownian motion are also negligible because of the low particle densities. Therefore, the deposition velocity and settling velocity are set to be 0 as model inputs.

5 Case Study – Results and Analysis

Model estimations from CALINE4, CAL3QHC and AERMOD at the Sacramento site, and from CALINE4 and CAL3QHC at the London site, were compared with measured concentrations. In order to see how the models performed, screen plots and statistical tests were used. For the sake of convenience, let D_{ij} (where i represents the model: 1 – CALINE4, 2 – CAL3QHC, and 3 – AERMOD; and j is the sample ID, $j = 1, 2, 3, \cdots$) denote the difference between the model-predicted concentrations and the observed concentrations.

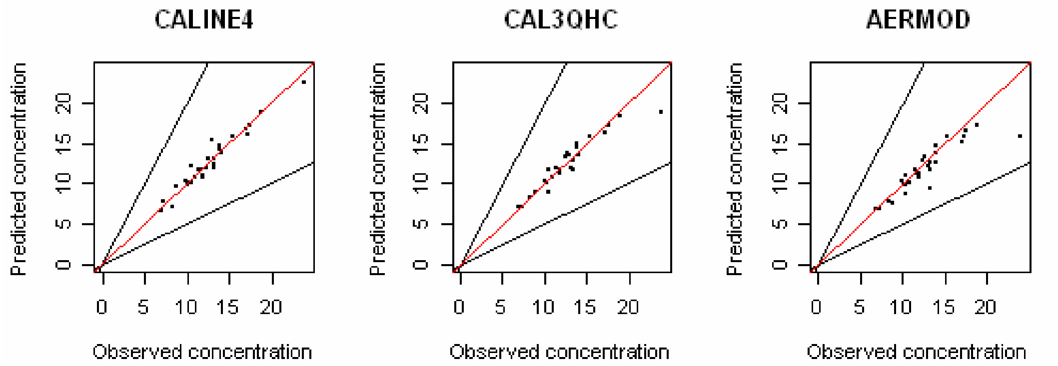
5.1 Screen Plots and Descriptive Statistics

5.1.1 Factor-of-Two Plots

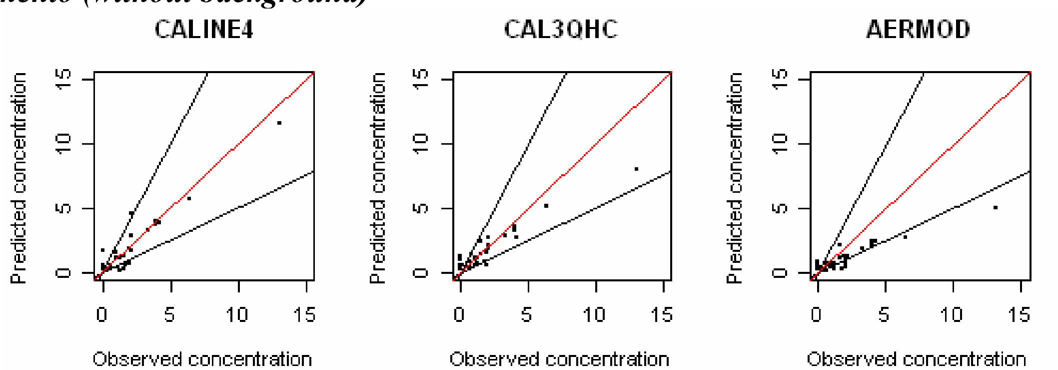
The "Factor-of-two" plot is a classical method to examine model performance. Typically, if 80% of the points fall inside the factor-of-two envelope, the model results are considered good in predicting true values (Yura et al., 2007, pp.8752).

Figure 5-1 and Table 5-1 show that all points are inside the factor-of-two envelope for both Sacramento and London sites when the background concentrations are included. However, when the background concentrations are not included, approximately half of the points are outside the factor-of-two envelope, suggesting that model results with CALINE4 and CAL3QHC do not match observed increments well, especially for the London site.

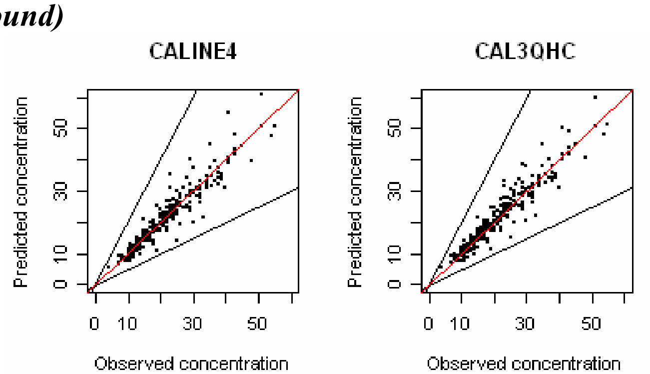
Sacramento (with background)



Sacramento (without background)



London (with background)



London (without background)

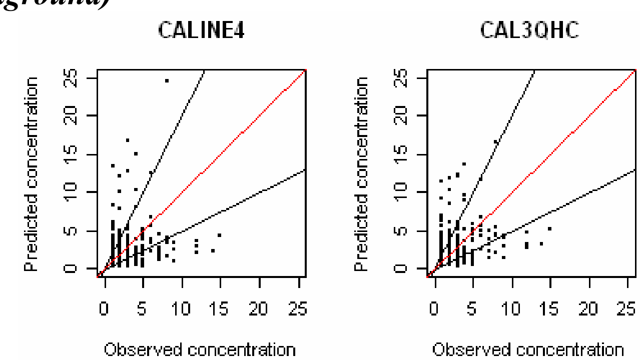


Figure 5-1 Factor-of-Two Plots (all concentrations are in μg/m³).

Table 5-1 Percentage of Points Falling in the Factor-of-two Envelope

	Sacramento		London	
	With background	Without background	With background	Without background
CALINE4	100%	59%	100%	57%
CAL3QHC	100%	69%	100%	59%
AERMOD	100%	48%	n/a	n/a

Note: AERMOD was not used for the London site due to limited available meteorological data.

It is important to note that, in this analysis, the factor-of-two plots can only serve as screening plots, rather than providing a conclusive argument regarding model effectiveness. In the plots with background, the difference between estimated concentration and observed concentration is masked by the background, especially when background concentrations are high. In the plots without background, points inside the envelope do not necessarily demonstrate that the predictions are good. For low increment concentrations, a point with good estimation may lie outside the envelope. For high increment concentrations, a point with bad estimation may still fall inside the envelope.

5.1.2 Difference Overview and Patterns

An explicit way to compare the model-estimated and observed concentrations is to look at their differences (D_{ij} s) and descriptive statistics. Differences close to zero indicate good model performance.

Table 5-2 shows that, for the Sacramento site, AERMOD produced the largest difference between model results and observed concentrations; CALINE4 and CAL3QHC performed better than AERMOD. The number counts of positive D_{ij} versus negative D_{ij} (TABLE 4 part (b)) suggest that the three models generally under-predicted concentrations.

Table 5-2 Difference Overview (values are in μg/m³).

(a) Basic Statistics

	D_{ij}			$\lvert D_{ij} \rvert$		D_{ij}^2	
	Sum	Min	Max	Sum	Average	Sum	Average
Sacramento Site (Sample Size = 29)							
CALINE4	-3.0	-1.5	2.3	18.2	0.628	20.6	0.710
CAL3QHC	-8.3	-5.1	1.2	21.3	0.734	40.5	1.397
AERMOD	-27.4	-8.1	0.8	34.3	1.182	106.4	3.668
London Site (Sample Size = 253)							
CALINE4	-74.9	-11.7	16.6	532.5	2.105	2790.0	11.028
CAL3QHC	20.9	-10.8	10.3	522.5	2.065	2331.7	9.216

where $\lvert D_{ij} \rvert$ denotes the absolute value of D_{ij}.

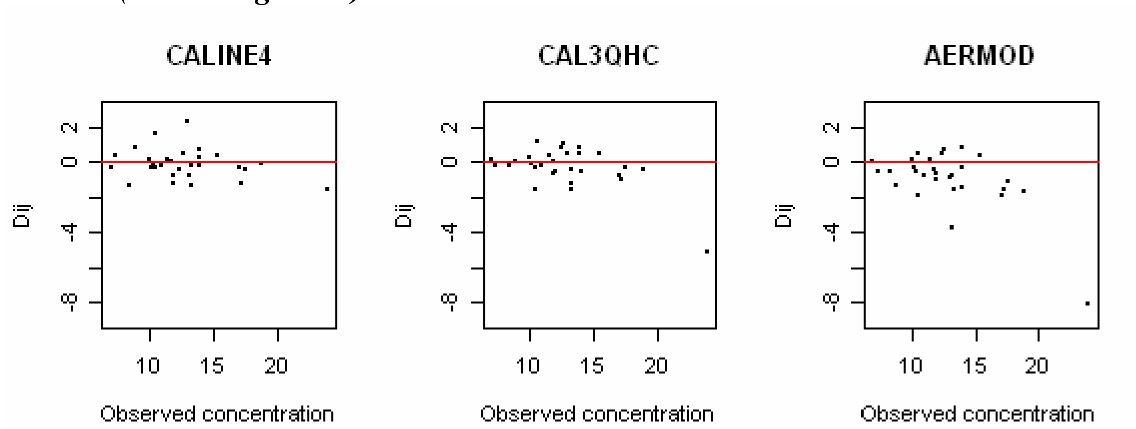
(b) Sample Number Count

	Sacramento (N = 29)			London (N = 253)		
	$D_{ij} < 0$	$D_{ij} = 0$	$D_{ij} > 0$	$D_{ij} < 0$	$D_{ij} = 0$	$D_{ij} > 0$
CALINE4	18	0	11	140	11	102
CAL3QHC	17	0	12	116	6	131
AERMOD	21	0	8	n/a	n/a	n/a

Note: AERMOD was not used for the London site due to limited available meteorological data.

We also plotted $\mathbf{D_{ij}}$ against observed concentrations to explore their patterns. As shown in Figure 5-2, when plotted without background concentrations (road increment only), most D_{ij}s are larger than zero when the observed concentration is small, and smaller than zero when the observed concentration is large. This suggests that model under-prediction increases with concentration. When plotted with observed concentration with background, the distribution of D_{ij} is almost symmetric around zero against the observed concentrations, and D_{ij}s seem to scatter more widely against higher observed concentrations. The different patterns shown in the two types of plots, with and without background, are due to the much higher background concentration than the increment concentrations.

Sacramento (with background)



Sacramento (without background)

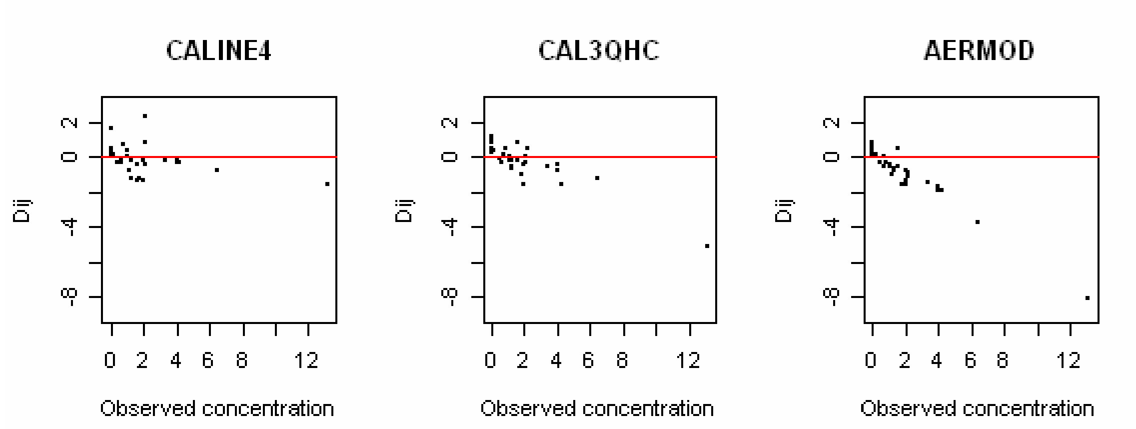
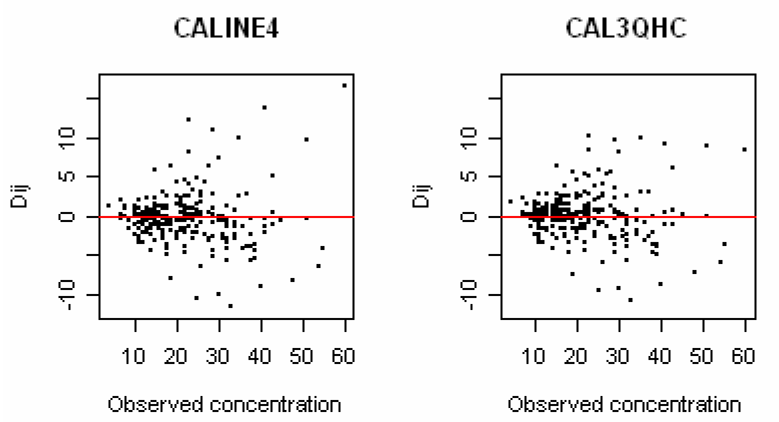


Figure 5-2 (part 1) Pattern of $\mathbf{D_{ij}}$ (all concentrations are in µg/m^3).

London (with background)



London (without background)

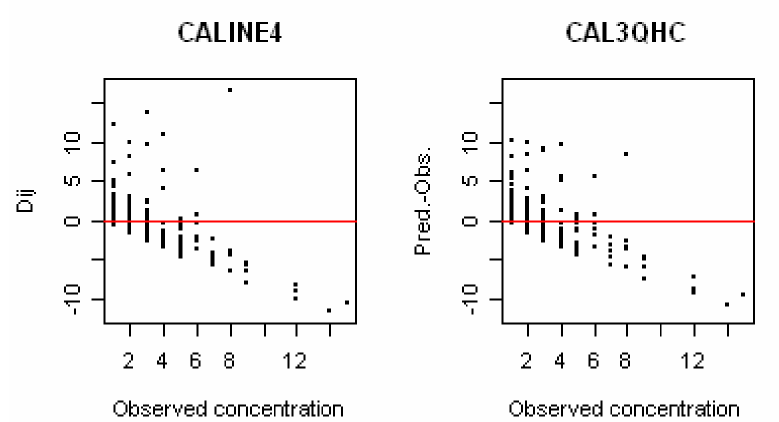


Figure 5-2 (part 2) Pattern of D_{ij} (all concentrations are in $\mu g/m^3$).

5.1.3 Correlation between Estimated and Observed Concentrations

In addition to plotting the differences, we also investigated the overall model performance based on the correlation between the estimated and observed concentrations. A high correlation is a necessary, though not sufficient condition of a good match between estimated and observed concentrations. R^2 quantitatively measures the correlation (see Table 5-3). The higher the R^2 value, the more the model-estimated and observed concentrations correlate.

Table 5-3 R^2 correlating model-predicted and observed concentrations.

	Sacramento		London	
	With background	Without background	With background	Without background
CALINE4	0.9454	0.8952	0.9009	0.0277
CAL3QHC	0.9044	0.8973	0.9134	0.0329
AERMOD	0.7905	0.8513	n/a	n/a

Note: AERMOD was not used for the London site due to limited available meteorological data.

In the Sacramento case, the correlations between estimated and observed concentrations are high for all three models in both with and without background scenarios. In the London case, the correlations are high for both models when the background concentrations are included; however, the correlations between estimated and observed concentrations without background are very small for both CALINE4 and CAL3QHC. Since the background concentrations are very high, the high correlations of both models in the London case are mostly due to the background (note that both model-predicted and observed total concentrations include the same background concentration for each data point).

5.2 Statistical Tests

We developed several statistical tests to investigate the following questions regarding the performance of CALINE4, CAL3QHC and AERMOD: a) Are the model-predicted $PM_{2.5}$ concentrations biased? b) Is there a trend of D_{ij} against observed concentrations? and c) Are there significant differences among the three models?

5.2.1 Test of Prediction Bias

We used the one-sample t-test to examine the hypothesis that the predicted concentrations provided by the three models are not biased. In order to perform the test, an assumption is made for D_{ij} that $D_{i1}, \cdots, D_{iN}$ (N is the sample size) are samples from a population with one distribution. As long as N is larger than 29, the central limit theorem can be applied and the one-sample t-test can be conducted. Both test statistic and p-value are calculated. A criterion of 0.05 for p-value is used; that is, if the p-value is smaller than 0.05, then we reject the hypothesis (i.e., the model is biased). In this particular case, we can also determine whether the model is under or over-predicting based on the sign of the test statistic. If the hypothesis is rejected, then a negative test statistic indicates under-predicting, while a positive test statistic suggests over-predicting.

Table 5-4 presents the test results. In the Sacramento case, model results from CALINE4 and CAL3QHC are not biased, while AERMOD under-predicts observed concentrations. For the London case, because Figure 5-2 indicates that the model results tend to over-predict for low increment concentrations and under-predict for high increment concentrations, the bias test was conducted using four categories: Category 1 (Increment concentration is 1 µg/m3), Category 2 (Increment concentration is 2 µg/m3), Category 3 (Increment concentration is 3 µg/m3), Category 4 (Increment concentration is larger than 3 µg/m3). The test statistics suggest that both CALINE4 and CAL3QHC over-predict for low increment concentrations and under-predict for high increment concentrations.

Table 5-4 Test Results for Prediction Bias.

(a) Sacramento Case (N = 29)

	T^*	p -value	Conclusion
CALINE4	-0.6643	0.512	Unbiased
CAL3QHC	-1.3281	0.195	Unbiased
AERMOD	-3.0004	0.0056	Under-Prediction

(b) London Case

	Category 1 (N = 74)			**Category 2 (N = 58)**		
	T^*	p -value	Conclusion	T^*	p -value	Conclusion
CALINE4	5.353	<0.0001	Over-Prediction	1.354	0.181	Unbiased
CAL3QHC	7.236	<0.0001	Over-Prediction	2.998	0.004	Over-Prediction
	Category 3 (N = 53)			**Category 4 (N = 68)**		
CALINE4	-0.302	0.764	Unbiased	-5.192	<0.0001	Under-Prediction
CAL3QHC	0.761	0.450	Unbiased	-5.461	<0.0001	Under-Prediction

Category 1 (Increment concentration is 1 µg/m3), Category 2 (Increment concentration is 2 µg/m3), Category 3 (Increment concentration is 3 µg/m3), Category 4 (Increment concentration is larger than 3 µg/m3).

5.2.2 Test of Prediction Trend

We conducted an alternate statistical test to explore the statistical significance of the trend that model under-prediction increases with increased concentration (i.e., D_{ij}s decrease with increasing increment concentrations, as shown in Figure 5-2). The hypothesis is that the slope of the regression between D_{ij} and the observed concentration is zero. If the test shows that the slope is significantly less than zero, then we can conclude a statistically significant trend. Table 5-5 shows that D_{ij}s decrease as the increment concentrations increase for all three models at both sites and the trend is statistically significant. However, when the background concentration is included, only CAL3QHC and AERMOD results at the Sacramento site show this trend.

Table 5-5 Test Result for Prediction Trend.

	With background			Without background		
	Estimated slope	p -value	Conclusion	Estimated slope	p -value	Conclusion
Sacrament site (N = 29)						
CALINE4	-0.062	0.167	D_{ij} →	-0.131	0.03	D_{ij} ↓
CAL3QHC	-0.176	0.002	D_{ij} ↓	-0.396	<0.0001	D_{ij} ↓
AERMOD	-0.287	0.0004	D_{ij} ↓	-0.628	<0.0001	D_{ij} ↓
London site (N = 253)						
CALINE4	-0.005	0.794	D_{ij} →	-0.806	<0.0001	D_{ij} ↓
CAL3QHC	-0.019	0.319	D_{ij} →	-0.816	<0.0001	D_{ij} ↓

where D_{ij} → means D_{ij} stays similar for different observed concentrations;

D_{ij} ↓ means D_{ij} becomes smaller when the observed concentration becomes larger (model under-prediction increases as concentrations increase).

For the Sacramento case (see Figure 5-2), there is one point whose increment concentration is larger than 12μg/m^3 (the increment concentrations for other points are all less than 6.5μg/m^3). Given the point's potential influence, we suspect that the trend may simply be caused by this one point for the Sacramento case. Statistical test results show that D_{ij}s decrease as the increments increase only for CAL3QHC and AERMOD, but not CALINE4 when this point is excluded. Since the increment concentrations of the remaining points are all less than 6.5μg/m^3, further studies are needed to evaluate the under-prediction trend with a larger spectrum of increment concentrations.

5.2.3 Test for Model Difference

In this section, the three models are compared by testing whether their estimates are statistically different from one another. Model results from the Sacramento site were used in this test and a one-factor ANOVA model was constructed. The ANOVA model specified D_{ij} s as the sample results and included one factor with three levels representing the three models (level 1 - CALINE4, level 2 - CAL3QHC, and level 3 - AERMOD). The sample size for each factor level is 29.

A hypothesis that the three models are not different from each other can be tested through a simultaneous 95% confidence interval for the three combinations of the differences between means of the three factor levels, $\mu_1 - \mu_2$, $\mu_1 - \mu_3$, and $\mu_2 - \mu_3$, where μ_1, μ_2 and μ_3 are the means of factor level 1, 2 and 3, respectively. Using the Bonferroni method, we can get confidence intervals between means of factor levels:

$\mu_1 - \mu_2$: [-0.642, 1.008]

$\mu_1 \quad \mu_3$: [0.015, 1.665]

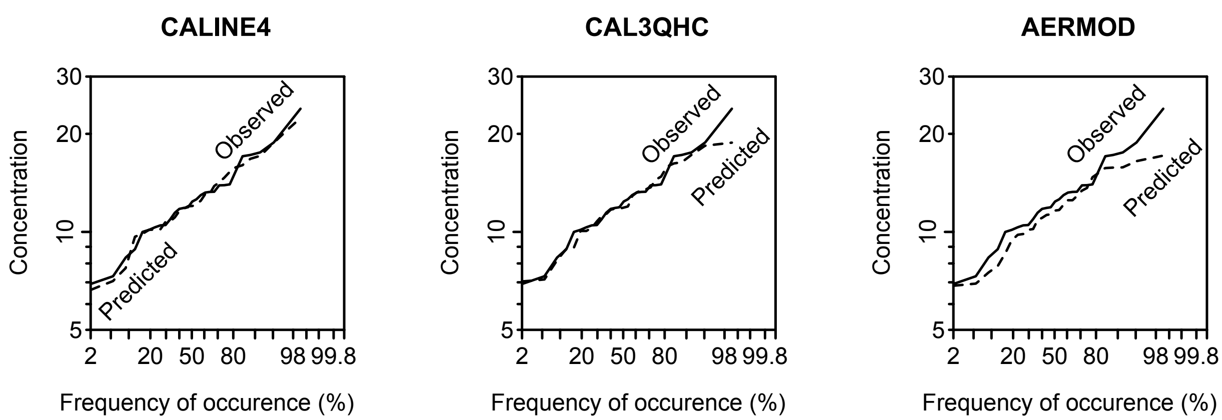
$\mu_2 - \mu_3$: [-0.168, 1.482]

Since both bounds of the interval of $\mu_1 - \mu_3$ are positive, the test suggests that predicted concentrations from AERMOD are significantly smaller than those provided by CALINE4 at the Sacramento site. This is consistent with the evidence in section 5.2.1 that AERMOD under-predicts $PM_{2.5}$ concentrations. The interval of $\mu_1 - \mu_2$ is almost symmetric around 0, which indicates that CALINE4 and CAL3QHC produce concentration estimates that are not statistically different from each other.

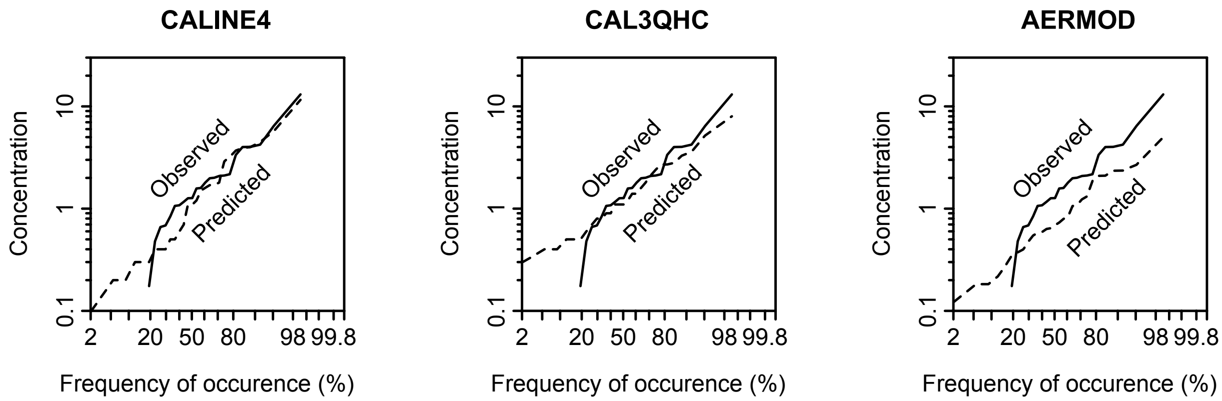
5.3 Distribution Patterns

The previous statistical comparisons assess the models' ability to simulate concentrations at a particular location at a particular time. They provide the most stringent tests of the models and establish what can be expected from air quality models with respect to their accuracy and precision. For some regulatory applications, it may not be crucial to accurately and precisely predict when and where a specific concentration may occur, such as determining compliance with an air quality standard. For this and similar purposes, the ability to adequately portray the distribution of concentrations occurring in an area unpaired in space and time may suffice. Cumulative frequency distribution plots of observed and predicted concentrations have been prepared to illustrate this (see Figure 5-3). Although these diagnostic plots provide a less stringent test of the models, the plots are useful for establishing visual patterns; i.e., systematic overestimations or underestimation of the observed distributions or even portions of the distributions, such as the highest concentrations.

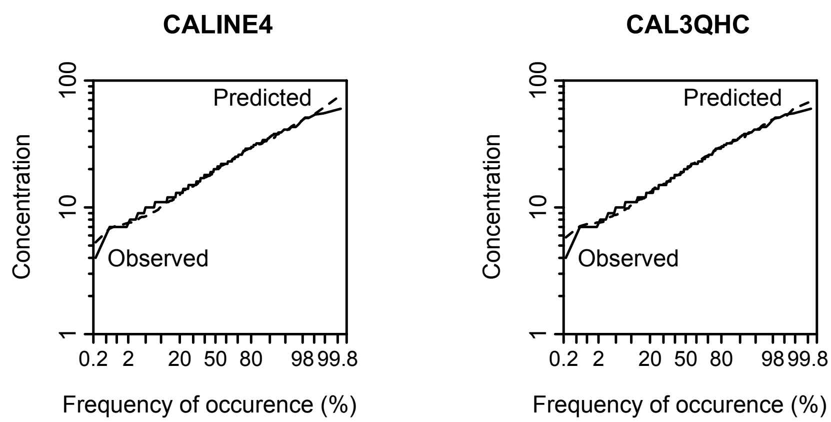
Sacramento (with background)



Sacramento (without background)



London (with background)



London (without background)

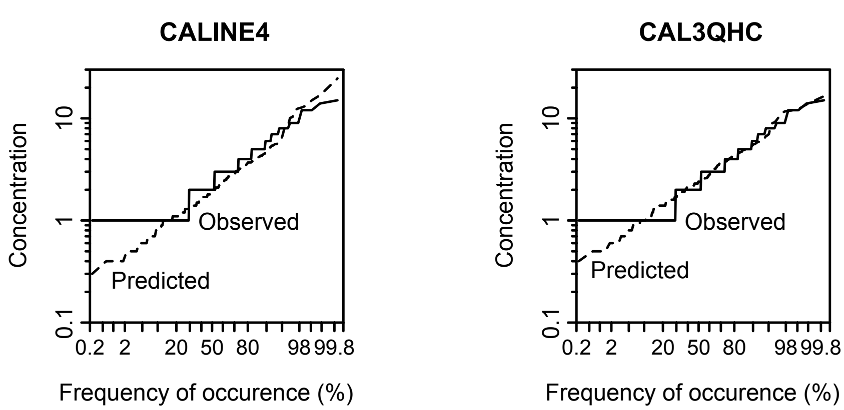


Figure 5-3 Cumulative Frequency Distributions of Observed Concentrations (solid lines) and Predicted Concentrations (dotted lines) (all concentrations are in μg/m³).

6 Discussion and Conclusion

In this study, when comparing predicted and observed concentrations, scenarios with and without background are considered. Screen plots and statistical tests show that different results may be concluded from the two scenarios.

In the Sacramento case, model results paired in space and time from CALINE4 and CAL3QHC match the observed concentrations moderately well, while AERMOD under-predicts $PM_{2.5}$ concentrations, based on a prediction bias test (section 5.2.1) and confidence intervals of the difference between means (section 5.2.3). All three models show a trend of under-predicting the observed values as the increment concentrations increase (section 5.2.2). When the data point with an increment concentration of 12μg/m^3 is excluded (all remaining data points are of increment concentrations less than 6.5μg/m^3), statistical test results show that D_{ij}s decrease as the increments increase only for CAL3QHC and AERMOD, but not for CALINE4. Therefore, further studies are needed to investigate how well the models perform across a larger spectrum of road-increment $PM_{2.5}$ concentrations.

In the London case, model results paired in space and time from CALINE4 and CAL3QHC do not match the observed concentrations (increments, without background). When the increment concentrations are small, both models over-predicted; for high increment concentrations, both models under-predicted. Both models showed a trend of predicting smaller than monitored values as the increment concentrations increased. In addition, when the backgrounds are excluded, the predicted concentrations behave as randomly chosen numbers against the observed concentration. The R^2 values also show little correlation between model results and measured concentrations when the backgrounds are excluded. There are two possible reasons for this bad match. First, the receptor at the London site is very close to the road segment. It is highly affected by instant nearby traffic and meteorological conditions. However, both models assume that the point for which the concentration is estimated achieves a steady state. This assumption is therefore not satisfied for the receptor location at the London site. Second, the street canyon effect may play an important role in PM dispersion at the London site. Since the study site includes numerous high buildings, the street canyon effect results in complex meteorology near the receptor. The comparison of London's results therefore indicates that CALINE4 and CAL3QHC are not suitable for estimating concentrations at places where stable state is not achieved.

Our comparative assessment suggests that AERMOD under-estimates near-road $PM_{2.5}$ concentrations at the Sacramento site. This is consistent with two previous studies that have shown under-predicted PM_{10} concentrations in AERMOD (Kesarkar et al., 2007; Zhang et al., 2008). Prior works, together with these findings, suggest that AERMOD may be inappropriate for estimating PM concentrations near roads. The evidence that AERMOD appears to under-predict concentrations, combined with the fact that more meteorological data and more user effort is required to run AERMOD, suggest that project-level analysts may want to run either CALINE4 or CAL3QHC as a first choice.

Note also, that theoretically, AERMOD can mimic real atmospheric conditions better; however, it requires more meteorological data to run, some of which can be difficult to obtain. (In the London case, AERMOD was not run because of limited available meteorological data.) Moreover, running AERMOD requires more user effort than the other two models due to the complexity of the model.

CAL3QHC has an optional queue algorithm. Using this algorithm may better simulate vehicle movements in signalized road segments. However, signal-related parameters and idle emission factors are needed in order to make use of the queue algorithm. In many cases, it is not easy to specify these parameters.

Another implication from this study is that factor-of-two plots are a limited resource for model evaluation. Factor-of-two plots have been a traditional test of model performance, and several previous studies have assessed model performance based solely or largely on the percentage of data points falling inside the factor-of-two envelope. As shown by this study, factor-of-two plots assist in screening-level assessments but lack the statistical detail offered by other tests.

Both the CALINE4 and CAL3QHC models accurately simulate the distribution of observed concentrations at the Sacramento and London sites. In the less rigorous comparison of predicted and observed concentrations unpaired in space and time, quite an improvement in model performances are indicated for the London site, with a slight advantage exhibited by the CAL3QHC model. Modelers should keep in mind, however, that this represents a compromised application case, where it is not important to determine when and where a specific concentration may occur. AERMOD tended to under-predict observed concentrations throughout most of the distribution as reflected in the statistical comparisons.

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Appendix A: Documentation of Steps to Complete Model Runs

A.1 CALINE4

Example input file (EX1.INP):

```
Sacramento
4PM2.5
100 0 0 0 3 2 1 1 1 0
D1 (3m)
D1 (9m)
D3 (3m)
18.3 19.4 3.0
18.3 19.4 9.0
74.5 75.6 3.0
Florin
Stockton
1 -150.0 0.0 150.0 0.0 0 32 0 0 0
1 -41.3 144.2 41.3 -144.2 0.0 28.0 0 0 0
11101Run 1
1919 1919
0.0692 0.0692
234.9 2.53 2 1000 15.8 0 34.88
```

Explanation of the input file

Table A- 1 CALINE4 Input Description

Line Number	Variable	Type	Unit	Example input	Description
1	Job title	Character		Sacramento	40 characters or less
2	Pollutant Type	Integer		4	1 = CO, 2 = NO_2, 3 = Inert Gas, 4 = Particulate
	Pollutant Name	Character		PM2.5	30 characters or less
3	Surface roughness	Real	cm	100.0	
	Molecular weight	Real		0[1]	
	Settling velocity	Real	cm/s	0	
	Deposition velocity	Real	cm/s	0	
	Number of receptors	Integer		3	
	Number of links	Integer		2	
	Scale factor	Real		1	Converts roadway geometry input variables to meters
	Link title option	Integer		1	0 = use default titles; 1 = specify titles by oneself.
	Receptor title option	Integer		1	0 = use default titles; 1 = specify titles by oneself.
	Altitude above sea level	Real		0	
4-6	Receptor name	Character		D1 (3m)	8 characters or less. (Only need to specify when 'Receptor title option' is 1. One row for one receptor.)
7-9	Receptor coordinates X, Y, Z	Real		18.3 19.4 3.0	One row for one receptor.
10-11	Link name	Character		Florin	12 characters or less. (Only need to specify when

[1] "CALINE4 initially computes all concentrations in mass per unit volume. These results are converted to a volumetric equivalent (i.e., parts per million) for gaseous pollutants." (Benson 1984, pp 49) 'Molecular weight' is only used in the converting process. When modeling PM, the concentrations in the output are in mass per unit volume, i.e., the converting process is not performed for modeling PM. Therefore, 'Molecular weight' is not involved in the modeling process for PM, and 0.0 is used. The same argument applies for 'Altitude above sea level'.

					'Receptor title option' is 1. One row for one receptor.)
12-13	Link type	Integer		1	1 = At-Grade, 2 = Depressed, 3 = Fill, 4 = Bridge, 5 = Parking Lot, 6 = Intersection.
	Link endpoint 1 corrdinates X, Y	Real		-150.0 0.0	
	Link endpoint 2 corrdinates X, Y	Real		150.0 0.0	
	Source height	Real		0	Should be within ±10m.
	Mixing zone width	Real		32	Width of traffic lane(s) plus 3 meters on each side. (The minimum allowable value is 10m.)
	Mixing width (right)	Real		0	0 is interpreted as no horizontal obstruction.
	Mixing width (left)	Real		0	0 is interpreted as no horizontal obstruction.
	Continuation code	Integer		0	Equals 1 if endpoint 1 of next link coincident with endpoint 2 of current link.
14	Run type	Integer		1	1 = Standard, 2 = Multi-run, 3 = Worst-case wind angle, 4 = Multi-run/worst-case hybrid, 9 = Multi-run (last run).
	Traffic volume code	Integer		1	Equals 0 if traffic volume on all links unchanged from previous run.
	Emission factor code	Integer		1	Equals 0 if emission factors for all links unchanged from previous run.
	Intersection parameter code	Integer		0	Equals 0 if intersection parameters unchanged from previous run. (In the example, no intersection parameters are specified, so 0 is used.)
	Meteorology code	Integer		1	Equals 0 if meteorology unchanged from previous run.
	Run title	Character		Run 1	12 characters or less.
15	Hourly traffic volumes by link	Real	veh/hr	1919	Lists in one row, different links separated by spaces.
16	Composite emission factors by link	Real	g/VMT	0.0692	Lists in one row, different links separated by spaces.

17	Wind direction	Real	degree	234.9	The direction the wind is blowing from, measured clockwise in degrees from the north. (This parameter is not used in calculation if "Worst-Case" is selected.)
	Wind speed	Real	m/s	2.53	
	Atmospheric stability class	Integer		2	Values 1 through 7 correspond to the standard definitions for stability class A through G.
	Mixing height	Real	m	1000	"Mixing height algorithm is primarily meant for study of special case nocturnal inversion, and may be bypass by assigning a value of 1000 meters or greater." (Benson, 1984)(pp.100)
	Wind direction standard deviation	Real	degree	15.8	
	Ambient concentration	Real	ppm	0	"The program automatically sums the contributions from each link to each receptor. After this has been completed for all receptors, an ambient value is added." (Benson, 1984) (pp.32) Therefore, the ambient concentration is not involved in the calculation of increment.
	Temperature	Real	°C	34.88	

Source: The description of input variables uses information from the technical report documentation of CALINE4 (Benson, 1984).

To execute the program, at the DOS prompt, go the directory with the executable program (caline4_50.exe) and the input file, type:

caline4_50 <input file name> output file name
For example: caline4_50 <EX1.INP> EX1.OUT

Example output file (EX1.OUT):

```
              CALINE4: CALIFORNIA LINE SOURCE DISPERSION MODEL
                      JUNE 1989 VERSION
                      PAGE   1

                 JOB: Sacramento
                 RUN: Run 1
           POLLUTANT: PM2.5
           (NOTE: OUTPUT IN MICRO-GRAMS/METER**3.  IGNORE PPM LABEL)

     I.  SITE VARIABLES

           U=   2.5 M/S             Z0= 100.  CM            ALT=     0.  (M)
         BRG= 234.9 DEGREES         VD=  0.0 CM/S
        CLAS=     2 (B)             VS=  0.0 CM/S
        MIXH= 1000.  M             AMB=  0.0 PPM
       SIGTH=   16.  DEGREES      TEMP= 34.9 DEGREE (C)


    II.  LINK VARIABLES

        LINK       *  LINK COORDINATES (M)   *              EF     H     W
     DESCRIPTION   *   X1    Y1    X2    Y2  * TYPE  VPH  (G/MI)  (M)   (M)
   ----------------*-------------------------*------------------------------
   A.  Florin      *  -150     0   150     0 *  AG   1919   0.1    0.0  32.0
   B.  Stockton    *   -41   144    41  -144 *  AG   1919   0.1    0.0  28.0


   III.  RECEPTOR LOCATIONS

                *    COORDINATES (M)
     RECEPTOR   *    X      Y      Z
   ------------*---------------------
   1.  D1 (3m)  *     18     19   3.0
   2.  D1 (9m)  *     18     19   9.0
   3.  D3 (3m)  *     75     76   3.0


    IV.  MODEL RESULTS (PRED.  CONC.  INCLUDES AMB.)

                * PRED  * CONC/LINK
                * CONC  *   (PPM)
    RECEPTOR    * (PPM) *   A    B
  -------------*-------*----------
   1.  D1 (3m)  *   3.9 *  2.3  1.6
   2.  D1 (9m)  *   0.4 *  0.3  0.1
   3.  D3 (3m)  *   1.5 *  0.9  0.6
```

A.2 CAL3QHC

Example input file (EX2.OUT):

```
'Sacramento 1'  60 100 0 0 3 1 0 0
'D1(3m)' 18.3 19.4 3.0
'D1(9m)' 18.3 19.4 9.0
'D3(3m)' 74.5 75.6 3.0
'number 1' 2 1 1 'P'
  1
'Florin'   'AG' 150.0 0.0   -150.0 0.0    1919  0.0692 0 32
  1
'Stockton' 'AG' -41.3 144.2 41.3   -144.2 1919  0.0692 0 28
2.53 234.9 2 1000 0  'Y' 16 -1 1
```

Explanation of the input file

Table A- 2 CAL3QHC Input Description

Line Number	Variable	Type	Unit	Example input	Description
1	'Job title'	Character		'Sacramento 1'	40 characters or less
	Averaging time	Real	min	60	Should be within the range of 30 min to 60 min.
	Surface roughness	Real	cm	100	
	Settling velocity	Real	cm/s	0	
	Deposition velocity	Real	cm/s	0	
	Number of receptors	Integer		3	Max = 60
	Scale factor	Real		1	Converts roadway geometry input variables to meters
	Metric conversion in output option	Integer		0	0 = output in meters, 1 = output in feet.
	Debugging option	Integer		0	0 = debugging option not wanted, 1 = input data echoed onto the screen, the echoing process stops when an error is detected.
2-4	'Receptor name'	Character		'D1 (3m)'	20 characters or less.

	Receptor coordinates X, Y, Z	Real		18.3 19.4 3.0	
5	Run title	Character		'Run 1'	40 characters or less.
	Number of links	Integer		2	Max = 120
	Number of meteorological conditions	Integer		1	Unlimited number.
	Output option	Integer		1	0 = summary output (short format), 1 = output that includes the receptor-link matrix tables (long format).
	'MODE'	Character		'P'	'C' = CO, 'P' = PM
6 & 8	IQ	Integer		1	1 = free flow, 2 = queue links.
7 & 9	'Link name'	Character		'Florin'	20 characters or less
	'Link type'	Character		'AG'	'AG' = at grade, 'FL' = fill, 'BR' = bridge, 'DP' = depressed.
	Link endpoint 1 corrdinates X, Y	Real		-150.0 0.0	
	Link endpoint 2 corrdinates X, Y	Real		150.0 0.0	
	Hourly traffic volumes by link	Real	veh/hr	1919	
	Composite emission factors by link	Real	g/VMT	0.0692	
	Source height	Real		0	Should be within ±10m.
	Mixing zone width	Real		32	Width of traffic lane(s) plus 3 meters on each side.
10	Wind speed	Real	m/s	2.53	
	Wind direction	Real	degree	234.9	The direction the wind is blowing from, measured clockwise in degrees from the north.
	Atmospheric stability class	Integer		2	Values 1 through 7 correspond to the standard definitions for stability class A through G.
	Mixing height	Real	m	1000	"Mixing height should be generally set at 1000m."(USEPA, 1995, pp.34)
	Ambient concentration	Real	ppm	0	Same explanation as in CALINE4.

	'Wind direction variation'	Character		'Y'	'Y' = allow wind direction to vary, 'N' = use only the specified wind direction.
	Wind direction increment angle	Integer		16	These three variables are not used in the case that 'N' is specified for 'Wind direction variation'; however, these three variables have to be specified in order for the program to run. If 'Y' is specified for 'Wind direction variation', concentration under wind direction from first increment to last increment will be displayed in the output.
	First increment multiplier	Integer		-1	
	Last increment multiplier	Integer		1	

Source: The description of input variables uses information from the User's Guide to CAL3QHC (USEPA, 1995).

To execute the program, at the DOS prompt, go the directory with the executable program (CAL3QHC.exe) and the input file, type:

CAL3QHC input file name output file name
For example: CAL3QHC EX2.INP EX2.OUT

Example output file (EX2.OUT):

```
      CAL3QHC: LINE SOURCE DISPERSION MODEL - VERSION 2.0 Dated 95221           PAGE  1

  JOB: Sacramento 1                              RUN: Run 1

  DATE :  6/23/ 8
  TIME :  1:20:38

    The MODE flag has been set to P for calculating PM averages.

   SITE & METEOROLOGICAL VARIABLES
   -------------------------------
   VS =   0.0 CM/S       VD =   0.0 CM/S       Z0 = 100.  CM
   U =  2.5 M/S    CLAS =   2  (B)    ATIM =  60.  MINUTES    MIXH =  1000.M   AMB =  0.0 ug/m**3

   LINK VARIABLES
   --------------
 LINK DESCRIPTION * LINK COORDINATES (M)  *   LENGTH BRG TYPE VPH    EF     H     W V/C QUEUE
```

```
                     *  X1     Y1     X2      Y2  *     (M)   (DEG)          (G/MI) (M) (M)      (VEH)
------------------------*--------------------------------*---------------------------------------------------------
 1.  Florin             * 150.0    0.0  -150.0     0.0 *    300.  270.  AG   1919.  0.1   0.0 32.0
 2.  Stockton           *  -41.3 144.2    41.3 -144.2 *    300.  164.  AG   1919.  0.1   0.0 28.0
```


JOB: Sacramento 1 RUN: Run 1

DATE : 6/23/ 8
TIME : 1:20:38

```
RECEPTOR LOCATIONS
------------------
                     *         COORDINATES (M)        *
   RECEPTOR          *        X         Y         Z         *
-------------------------*-----------------------------------------*
 1.  D1(3m)           *       18.3      19.4       3.0          *
 2.  D1(9m)           *       18.3      19.4       9.0          *
 3.  D3(3m)           *       74.5      75.6       3.0          *
```

MODEL RESULTS

REMARKS : In search of the angle corresponding to
the maximum concentration, only the first
angle, of the angles with same maximum
concentrations, is indicated as maximum.

WIND ANGLE RANGE: 219.-251.

```
WIND     * CONCENTRATION
ANGLE   *     (ug/m**3)
(DEGR)   * REC1  REC2  REC3
------------*--------------------------
219.        *    3.      1.       1.
235.        *    3.      1.       1.
251.        *    3.      1.       1.
------------*---------------------------
MAX       *    3.      1.       1.
DEGR.   *  234     218     218
```

THE HIGHEST CONCENTRATION OF 3. ug/m**3 OCCURRED AT RECEPTOR REC1 .

JOB: Sacramento 1 RUN: Run 1

DATE : 6/23/ 8
TIME : 1:20:38

RECEPTOR - LINK MATRIX FOR THE ANGLE PRODUCING
THE MAXIMUM CONCENTRATION FOR EACH RECEPTOR

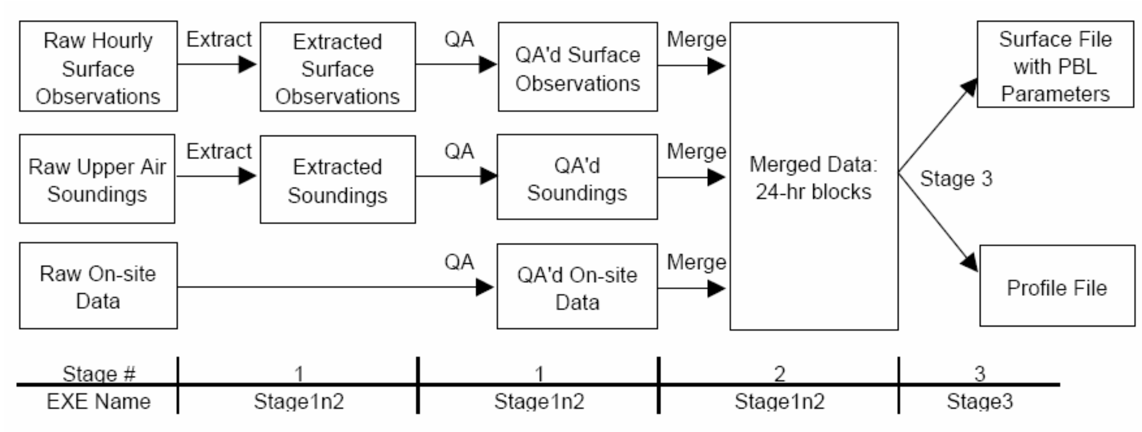
```
           *    PM/LNK(ug/m**3)
           *    ANGLE (DEGREES)
           *  REC1  REC2  REC3
 LINK #    *   234   218   218
-----------*----------------------------
    1      *   1.4   0.4   0.5
    2      *   1.3   0.4   0.4
```

We can get the predicted $PM_{2.5}$ concentration in 'PAGE 3' of the output file.

A.3 AERMOD

Before running AERMOD, two meteorological data files should be prepared first by AERMET.

The basic process of AERMET is displayed in the following figure.



Source: this figure is reproduced from the User's Guide for AERMET (USEPA, 2004c).

Figure A- 1 AERMET Process

In stage 1, AERMET extracts Raw Hourly Surface Observations and Raw Upper Air Soundings from standard National Climatic Data Center (NCDC) formats. Then quality assessment will be performed on these data and Raw On-site data. These data are merged in stage 2. AERMET generates two meteorological data files based on these data in stage 3. The two meteorological data files are used as inputs for AERMOD.

Because we do not have Hourly Surface Observations or Upper Air Soundings in standard NCDC formats and the NCDC formats are specially coded, we generate two files in formats that can be used as inputs for stage 2 directly. For example, in the Sacramento case, two files, SAC_SF.OQA and SAC_UA.OQA are generated (Table A-3). ('SF' denotes 'Surface observation', 'UA' denotes 'Upper Air soundings', and 'OQA' denotes 'Output from Quality Assessment'.) 95082312 -9 99999 99999 999 0099 09999 09999 09999 09999 09999 09999

9999 9999 99 999 99999 349 999 999 24 23 25

Table A- 3 Explanation of Surface Observation Input for Stage 2

Line	Variable	Example Input	Description	Missing indicator	Lower bound	Upper bound
1	Hour	95082312	Year (2 digits), month (2 digits), day (2 digits), hour[1] (2 digits) of the local standard time[2].			
	PRCP	-9	Precipitation amount (millimeters), multiplied by 1000.	-9	0	25400
	SLVP	99999	Sea level pressure (millibars), multiplied by 10.	99999	9000	10999
	PRES	99999	Station pressure (millibars), multiplied by 10.	99999	9000	10999
	CLHT	999	Ceiling height (kilometers), multiplied by 10.	999	0	300
	TSKC	0099	Total sky cover[3] (code, 2 digits), opaque sky cover (code, 2 digits). (In this case, total sky cover is clear and opaque sky over is missing.)	9999	0	1010
	C2C3	09999	0, Sky cover 2 layers (code, 2 digits), Sky cover 3 layers (code, 2 digits).	09999		
	CLC1	09999	0, Sky condition (code, 2 digits), Sky coverage (code, 2 digits), layer 1.	09999		
	CLC2	09999	0, Sky condition (code, 2 digits), Sky coverage (code, 2 digits), layer 2.	09999		
	CLC3	09999	0, Sky condition (code, 2 digits), Sky coverage (code, 2 digits), layer 3.	09999		
	CLC4	09999	0, Sky condition (code, 2 digits), Sky coverage (code, 2 digits), layer 4.	09999		
2	CLT	09999	0, Cloud type (code, 2 digits), height (tenths of kilometers, 2 digits).	09999		
	PWVC	9999	Present weather	9999	0	9800

[1] Hour '01' represents the time slot from 0:00am to 1:00am, and so on.
[2] Local Standard Time is the time without daytime saving in this case.
[3] Sky condition code: 00 – clear or less than 0.1 coverage; 01 – thin scattered 0.1 to 0.5 coverage; 02 – scattered 0.1 to 0.5 coverage; 03 – thin broken 0.6 to 0.9 coverage; 04 – broken 0.6 to 0.9 coverage; 05 – thin overcast 1.0 coverage; 06 – overcast 1.0 coverage; 07 – obscuration 1.0 coverage; 08 – partial obscuration <1.0 coverage; 09 – unknown.

	PWTH	9999	Precipitation type	9999	0	9800
	ASKY	99	ASOS sky condition, divided by 10.	99	0	10
	ACHT	999	ASOS ceiling (kilometers), multiplied by 10.	999	0	888
	HZVS	99999	Horizontal visibility (kilometers), multiplied by 10.	99999	0	1640
	TMPD	349	Dry bulb temperature (^oC), multiplied by 10. (In this case, the dry bulb temperature is 34.88, multiplied by 10 gives 348.8 and the nearest integer is 349.)	999	-300	360
	TMPW	999	Wet bulb temperature (^oC), multiplied by 10.	999	-650	350
	DPTP	999	Dew-point temperature (^oC), multiplied by 10.	999	-650	350
	RHUM	24	Relative humidity (percent)	999	0	100
	WDIR	23	Wind direction (degree), divide by 10. (In this case, the wind direction is 234.9, divided by 10 given 23.49 and 23 is the nearest integer.)	999	0	36
	WSPD	25	Wind speed (m/s), multiplied by 10. (the actual wind speed is 2.5m/s in this situation.)	999	0	500

Source: The descriptions of input variables, missing indicators, lower bounds and upper bounds use information from the User's Guide for AERMET(USEPA, 2004c).

The following gives a base unit of the 'Upper Air Observation' input file for stage 2 by showing the upper air sounding information of August 23, 1995. For each variable, integers are used (numbers with decimals will cause the executable file to fail). For the complete file, the upper air characteristics of every day from August 23 to 26 are listed. (The explanation of the base unit is shown in Table A- 4.)

```
95082304   16
  10130       6    150    130    270     30
  10000     115    145    135    262     30
   9250     785    258    -27    279     40
   8500    1522    217     24    204     40
   7000    3166     91   -146    192    110
   5000    5869    -49   -290    222     80
   4000    7586   -165   -376    252     60
   3000    9684   -318   -502    233    140
   2500   10945   -410   -573    230    130
   2000   12431   -507   -655    225    150
   1500   14246   -647   -770    225    190
   1000   16681   -693   -806    222     90
    700   18831   -645   -768    207     50
    500   20910   -610   -738    157     20
    300   24158   -525   -670     84     90
    200   26799   -486   -637     91     70
```

Table A- 4 Explanation of Upper Air Sounding Input for Stage 2

Line	Variable	Example input	Description
1	Hour	95082304	Year (2 digits), month (2 digits), day (2 digits), hour (2 digits) of the local standard time.
	Level number	16	Number of levels in this sounding
2-17	UAPR	10130	Atmospheric pressure (millibars), multiplied by 10.
	UAHT	6	Height above ground level (meters).
	UATT	150	Dry bulb temperature (^{o}C), multiplied by 10.
	UATD	130	Dew-point temperature (^{o}C), multiplied by 10.
	UAWD	270	Wind direction (degrees from north).
	UAWS	30	Wind speed (m/s), multiplied by 10.

Source: The descriptions of input variables use information from the User’s Guide for AERMET(USEPA, 2004c).

Input file for Running Stage 2 (AERMET2.INP):

```
JOB
    REPORT     SAC_S2.RPT     # File records all messages
    MESSAGES   SAC_S2.MSG     # File records run summary

UPPERAIR
    QAOUT      SAC_UA.OQA     # Input file with Surface Observations

SURFACE
    QAOUT      SAC_SF.OQA     # Input file with Upper Air Soundings

MERGE
    OUTPUT     SAC_MR.MET     # Output file with merged data

    XDATES     95/08/23 95/08/26    # Time period included in the
output
```

Texts after # are explanations, and the explanations are not included in the file for execution.

To execute AERMET2.INP, put AERMET2.INP, SAC_UA.OQA, SAC_SF.OQA and AERMET.exe in the same folder, change AERMET2.INP to AERMET.INP, double click AERMET.exe, then three files will be generated (their names are specified in the AERMET2.INP): SAC_S2.RPT, SAC_S2.MSG, and SAC_MR.MET, where SAC_MR.MET is the merged file.

Input file for running stage 3 (AERMET3.INP):

```
JOB
    REPORT    SAC_S3.RPT      # File records all messages
    MESSAGES  SAC_S3.MSG      # File records run summary

METPREP
    DATA      SAC_MR.MET      # Input meteorological data

    OUTPUT    SAC_MP.SFC      # Output file with boundary laywer
    PROFILE   SAC_MP.PFL      # Output file with profile data

    LOCATION  OAK 122.22W 37.75N 8

    METHOD    REFLEVEL  SUBNWS
    NWS_HGT   WIND      6.1
    FREQ_SECT ANNUAL 1
    SECTOR    1    0     360
    SITE_CHAR 1 1  0.16  2.0  1
```

Texts after # are explanations, and the explanations are not included in the file for execution.

The last six lines are explained in Table A- 5.

Table A- 5 Explanation of Part of AERMET3.INP

Line	Variable	Example input	Description
LOCATION	Name	OAK	The name of station where the upper air sounding data are from.
	Location	122.22W 37.75N	Longitude and latitude of the station.
	Factor	8	The factor to convert local standard time to GMT[1].
METHOD		REFLEVEL SUBNWS	To substitute NWS data in the computations when there is no site-specific data.
NWS_HGT		WIND 6.1	The height at which the wind is measured. (here 6.1m)
FREQ_SECT	Time Frequency	ANNUAL	Annual – one frequency; Seasonal – four frequencies; Monthly – twelve frequencies.

[1] GMT is the Greenwich Mean Time. The factor to convert Local Standard Time of station 'OAK' to GMT is 8.

	Wind Sector	1	Number of wind sectors, at least 1, at most 12.
SECTOR	Sector ID	1	
	Wind range	0 360	Wind ranges from all wind sectors add to cover the full circle.
SITE_CHAR	Frequency ID	1	
	Sector ID	1	
	Midday albedo	0.16	Referring to Table 4-1 in the User's Guide for AERMET(USEPA, 2004c)
	Daytime Bowen ratio	2.0	Referring to Table 4-2b in the User's Guide for AERMET(USEPA, 2004c)
	Surface roughness length (meters)	1	Referring to Table 4-3 in the User's Guide for AERMET(USEPA, 2004c)

To execute AERMET3.INP, put AERMET3.INP, SAC_MR.MET and AERMET.exe in the same folder, change AERMET3.INP to AERMET.INP, double click AERMET.exe, then four files will be generated (their names are specified in the AERMET2.INP): SAC_S3.RPT, SAC_S3.MSG, SAC_MP.SFC and SAC_MP.PFL, where SAC_MP.SFC and SAC_MP.PFL are meteorological input files for AERMOD.

Input file for Running AERMOD (AERMOD.INP):

```
CO STARTING                   # Start of Control Pathway
   TITLEONE Sacramento        # Main title of the run
   MODELOPT  CONC   FLAT
   AVERTIME  1                # 1 hour average will be calculated
   POLLUTID  PM               # Pollutant type is PM
   FLAGPOLE  3.0
   RUNORNOT  RUN              # Run the model regardless the any errors
   ERRORFIL  ERRORS.OUT       # File records errors
CO FINISHED                   # End of Control Pathway

SO STARTING                   # Start of Source Pathway
   ELEVUNIT  METERS           # Specify the unit to be meters
   LOCATION  FLORIN1  AREA  -150.0 -16.0 0.0
```

```
   SRCPARAM  FLORIN1  0.000000716293 0.0 300.0 32.0 0
   LOCATION  STOCKT1  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT1  0.000000818621 0.0 300.0 28.0 74
   LOCATION  FLORIN2  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN2  0.000001411563 0.0 300.0 26.0 0
   LOCATION  STOCKT2  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT2  0.000001613214 0.0 300.0 22.0 74
   LOCATION  FLORIN3  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN3  0.000000702860 0.0 300.0 26.0 0
   LOCATION  STOCKT3  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT3  0.000000803269 0.0 300.0 22.0 74
   LOCATION  FLORIN4  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN4  0.000002401797 0.0 300.0 26.0 0
   LOCATION  STOCKT4  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT4  0.000002744911 0.0 300.0 22.0 74
   LOCATION  FLORIN5  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN5  0.000000724245 0.0 300.0 26.0 0
   LOCATION  STOCKT5  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT5  0.000000827708 0.0 300.0 22.0 74
   LOCATION  FLORIN6  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN6  0.000000249375 0.0 300.0 26.0 0
   LOCATION  STOCKT6  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT6  0.000000285000 0.0 300.0 22.0 74
   LOCATION  FLORIN7  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN7  0.000000703702 0.0 300.0 26.0 0
   LOCATION  STOCKT7  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT7  0.000000804231 0.0 300.0 22.0 74
   LOCATION  FLORIN8  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN8  0.000000168490 0.0 300.0 26.0 0
   LOCATION  STOCKT8  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT8  0.000000192560 0.0 300.0 22.0 74
   LOCATION  FLORIN9  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN9  0.000000215894 0.0 300.0 26.0 0
   LOCATION  STOCKT9  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT9  0.000000246736 0.0 300.0 22.0 74
   LOCATION  FLORIN10  AREA  -150.0 -16.0 0.0
   SRCPARAM  FLORIN10  0.000000160547 0.0 300.0 26.0 0
   LOCATION  STOCKT10  AREA  -54.8 140.3 0.0
   SRCPARAM  STOCKT10  0.000000183482 0.0 300.0 22.0 74
   SRCGROUP  GROUP1 FLORIN1 STOCKT1
   SRCGROUP  GROUP2 FLORIN2 STOCKT2
   SRCGROUP  GROUP3 FLORIN3 STOCKT3
   SRCGROUP  GROUP4 FLORIN4 STOCKT4
   SRCGROUP  GROUP5 FLORIN5 STOCKT5
   SRCGROUP  GROUP6 FLORIN6 STOCKT6
   SRCGROUP  GROUP7 FLORIN7 STOCKT7
   SRCGROUP  GROUP8 FLORIN8 STOCKT8
   SRCGROUP  GROUP9 FLORIN9 STOCKT9
   SRCGROUP  GROUP10 FLORIN10 STOCKT10
SO FINISHED                   # End of Source Pathway

RE STARTING                   # Start of Receptor Pathway
   DISCCART 18.3 19.4 3.0     # x,y,z coordinates of receptor 1
```

```
   DISCCART 18.3 19.41 9.0    # x,y[1],z coordinates of receptor 2
   DISCCART 74.5 75.6 3.0     # x,y,z coordinates of receptor 3
RE FINISHED                   # End of Receptor Pathway

ME STARTING                   # Start of Meteorology Pathway
   SURFFILE  SAC_MP.SFC       # Input file with Surface Observations
   PROFFILE  SAC_MP.PFL       # Input file with Upper Air Soundings
   SURFDATA  0  1995  OAK,CA  # Surface meteorological station info.
   UAIRDATA  0  1995  OAK,CA  # Upper Air meteorological station info.
   SITEDATA  0  1995          # Site-specific meteorological station info.
   PROFBASE  0.0  METERS      # Specifies the base elevation above MSL[2]
ME FINISHED                   # End of Meteorology Pathway

OU STARTING                   # Start of Output Pathway
   MAXTABLE  ALLAVE  300      # Output the first 300 concentrations[3]
OU FINISHED                   # End of Output Pathway
```

Texts after # are explanations, and the explanations are not included in the file for execution.

Lines without explanations are explained in Table A- 6.

Table A- 6 Explanation of Part of AERMOD.INP

Line	Variable	Example input	Description
CO - MODELOPT		CONC	“Specifies that concentration values will be calculated.”
		FLAT	“Specifies that non-default option of assuming flat terrain will be used.”
CO - FALGPLOE		3.0	Specifies the default receptor height. If the receptor height is specified in the Receptor pathway, it will override the default value given here.
SO - LOCATION	Name	FLORIN1	Name of the source
	Type	AREA	Type of the source
	Location	-150.0 -16.0 0.0	x,y,z-coordinates of the source. The point of the source is determined referring to Figure 3-1 in the User’s Guide for AERMOD (USEPA, 2004a).

[1] The y-coordinate of receptor is modified from 19.4 to 19.41. The reason is that the output uses x,y-coordinates to distinguish receptors, and receptor 1 and 2 will be of no difference. The modification is done to make them differ from each other while it is not affect the outputs for receptor 2.

[2] MSL = Mean Sea Level

[3] 300 is used because the output will then cover all receptors throughout every hour of the 4 days (3 receptors * 96 hours <300).

SO – SRCPARAM	Name	FLORIN1	
	Area emission rate in g/(s-m^2)	0.000000716293	
	Source height	0.0	
	Xinit	300.0	Length of X side of the area
	Yinit	32.0	Length of Y side of the area
	Angle	0.0	"Orientation angle for the rectangular area in degrees from North, measured positive in the clockwise direction."
SO - SRCGROUP	Group Name	GROUP1	The output will give PM concentration from each group.
	Sources	FLORIN1 STOCKT1	Sources considered in the group.

To execute AERMOD.INP, put AERMOD.INP, SAC_MP.SFC, SAC_MP.PFL and AERMET.exe in the same folder, double click AERMET.exe, then two files will be generated (their names are specified in AERMOD.INP): ERRORS.OUT and AERMOD.OUT. We can get the predicted $PM_{2.5}$ concentrations in AERMOD.OUT.

Appendix B: Abbreviations

AERMET = AERmod's METeorological data preprocessor (a meteorological data preprocessor for AERMOD)

AERMOD = American Meteorological Society (Ams) and U.S. Environmental Protection Agency (Epa) Regulatory MODel

CAL3QHC = CALINE3 with Queuing and Hot-spot Calculations

CALINE3 = California LINE source dispersion model version 3

CALINE4 = California LINE source dispersion model version 4

CBL = Convective Boundary Layer

EPA = Environmental Protection Agency

GMT = Greenwich Mean Time

MSL = Mean Sea Level

PM = Particulate Matter

$PM_{2.5}$ = Particulate Matter less than 2.5 µm

PM_{10} = Particulate Matter less than 10 µm

PBL = Planetary Boundary Layer

SBL = Stable Boundary Layer